AFRL-RI-RS-TR-2009-179
In-House Interim Report
July 2009

SIMULATION CONCEPT – HOW TO EXPLOIT TOOLS FOR COMPUTING HYBRIDS

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FOR THE DIRECTOR:

/s/
MICHAEL J. HAYDUK
Branch Chief

/s/
EDWARD J. JONES, Deputy Chief
Advanced Computing Division
Information Directorate

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
JULY 2009	Interim	January 2007 – January 2009

4. TITLE AND SUBTITLE

SIMULATION CONCEPT – HOW TO EXPLOIT TOOLS FOR COMPUTING HYBRIDS

5a. CONTRACT NUMBER
In-House 459TSCHE

5b. GRANT NUMBER
N/A

5c. PROGRAM ELEMENT NUMBER
62702F

6. AUTHOR(S)

Clare D. Thiem and Joseph M. Hertline

5d. PROJECT NUMBER
459T

5e. TASK NUMBER
SC

5f. WORK UNIT NUMBER
HE

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

AFRL/RITC
525 Brooks Rd.
Rome NY 13441-4505

8. PERFORMING ORGANIZATION REPORT NUMBER
N/A

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

AFRL/RITC
525 Brooks Rd.
Rome NY 13441-4505

10. SPONSOR/MONITOR'S ACRONYM(S)
N/A

11. SPONSORING/MONITORING AGENCY REPORT NUMBER
AFRL-RI-RS-TR-2009-179

12. DISTRIBUTION AVAILABILITY STATEMENT
APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED. PA# 88ABW-2009-3133 Date Cleared: 14-July-2009

13. SUPPLEMENTARY NOTES

14. ABSTRACT
The Simulation Concept – How to Exploit Tools for Computing Hybrids (SCHETCH) project is exploring the design modeling and simulation (M&S) process for developing advanced computing technology for future intelligent systems. The desire is to integrate new alternative computing concepts with existing silicon-based computing technology in hybrid computing architectures. This interim report documents what progress has been made during the first two years of the effort. Literature reviews, past modeling and simulation experience, and current first hand modeling and simulation experience were all leveraged for this project. During this effort several alternative computing concepts were examined. A modeling and simulation process for the design and development of hardware implementation of alternative computing concepts was defined. Commercially available software was found to be applicable in the examination of components of quantum computing concepts. This success is being transitioned to support other in-house efforts pursuing quantum computing. Technology gaps were identified.

15. SUBJECT TERMS
Design, Modeling, Simulation, Computing, Finite Element Analysis, Parametric Modeling, Microelectromechanical Systems, MEMS, Nanoelectromechanical Systems, NEMS, Quantum Computing, Nanotechnology

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Clare D. Thiem
U	U	U	UU	53	19b. TELEPHONE NUMBER (*Include area code*) N/A

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1.0 INTRODUCTION

The Simulation Concept – How to Exploit Tools for Computing Hybrids (SCHETCH) project is exploring the design modeling and simulation (M&S) process for developing advanced computing technology for future intelligent systems. It represents a necessary step in the broader Air Force Research Laboratory's (AFRL's) research and development (R&D) activity which seeks to provide new warfighting capabilities to the Air Force. A main premise behind this project is that, for an alternative computing concept to move from laboratory novelty to a technology ready for the field, the proper M&S process must be in place. This requires some understanding as to whether or not existing M&S tools and techniques can be applied to the new technology or if new M&S paradigms need to be developed. Adaptation and integration of commercially-available software provides an opportunity to take advantage of existing functionality without investing time into developing new tools for new concepts. Thus, if the tools and techniques are well defined for modeling a technology then the technology's maturity level is at a point where the broader community can begin to explore ways to exploit it. The number of alternative computing concepts, however, is too large for this project to address all of them. Therefore, it was decided to focus on "hardware" concepts and not software implementations. A decision was also made to initially look at only three concepts: nanomechanical quantum computing, membrane computing, and deoxyribonucleic acid (DNA) computing. This report provides an overview of progress that has been made since the project started. The design M&S process was explored utilizing a combination of literature reviews, discussions, and modeling and simulation trade studies leveraging past experience whenever possible. During this examination some effort was made to identify limitations of existing M&S technology. Naturally, as the project progressed, and the directorate's and division organizational focus evolved, adjustments were made. These adjustments will be explained at the appropriate places throughout the report. This report starts by providing additional background information for the project then moves on to discuss M&S issues related to nanotechnology, biotechnology and approaches to quantum computing. Along the way technology gaps will be identified before wrapping up with some closing remarks.

2.0 BACKGROUND

One research thrust of the Advanced Computing Architectures Core Technical Competency (CTC) Area when this effort began was to examine novel information processing paradigms. [1] Over the past several years members of the Advanced Computing Division have supported several Defense Advanced Research Projects Agency (DARPA) Programs that fall under the broad category of biotechnology and quantum sciences. These programs were designed to demonstrate the integration of bio-fluidics with electronics (Bio-Fluidic Chips - BioFlips), expand the capability of multiphysics design tools (Simulation of Biological Systems - SIMBIOSYS), provide an open source environment for biological simulation tools (Bio-Computation - BioCOMP), and examine quantum computing architectures and algorithms (Quantum Information Science and Technology - QuIST). The results of these programs will play a role in demonstrating how biotechnology and quantum sciences can provide new capabilities for information dominance. Before the capability of a biologically-based or quantum-based information system concept can be demonstrated, however, more research is required to develop the technology to the level of maturity commensurate with practical application. The previous project, Establishing Tools for Computing Hybrids (ETCH), examined roles for which biotechnology could be leveraged for information dominance. ETCH determined that computational biology tools do have a role in maturing the technology, and showed that tools in the Biological Simulation Program for Intra-Cellular Evaluation (Bio-SPICE) software environment could be used in the development of bio-molecular computing concepts. [2] ETCH did not examine the quantum aspects of hybrid architectures. The basic question, as illustrated in Figure 1, is how do you bring new science into existing M&S process? Will existing M&S paradigms work, or a new ones required? The baseline for multi-physics, multi-scale M&S is the process that was developed under the DARPA Design for Mixed Technology Integration Program, shown in Figure 2 below, which was used by the AFRL in-house team during its baseline effort.

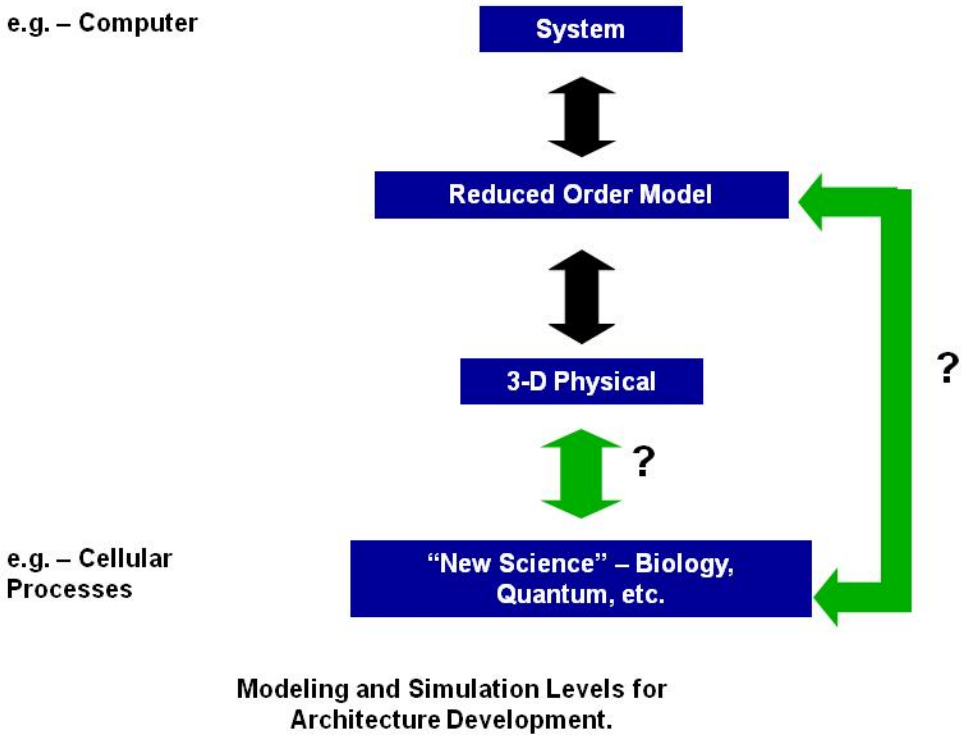


Figure 1: Graphical representation of basic question behind this project

Figure 3 illustrates the process that will be pursued for this project utilizing specific commercially available tools. The geometry is introduced in a computer-aided design (CAD) environment. CAD software for three-dimensional model generation allows for the establishment of geometry and physical characteristics of the desired structure. SolidWorks is a parametric CAD package, meaning it allows for manipulation of features such as dimensions or constraints to change the relationships in a single part, or in an assembly of components. This is useful in the design process where ideas are often refined and physical characteristics and geometry relationships change. A model can easily be updated by changing constraints and dimensions without starting from the very beginning of the model generation process. Similarly, visualization in this step of the design process also allows for clear communication of ideas to the user and their audience. SolidWorks allows for material assignment to components in assemblies. This is often useful in electronics because of differing materials such as copper and silicon. Finally, SolidWorks offers a variety of file formats for saving a model that is created, allowing for versatility and compatibility with a number of different programs for viewing, importing, manipulation and analysis of the model generated. For this particular effort three-dimensional physical model geometry from SolidWorks can be imported into COMSOL Multiphysics for analysis.

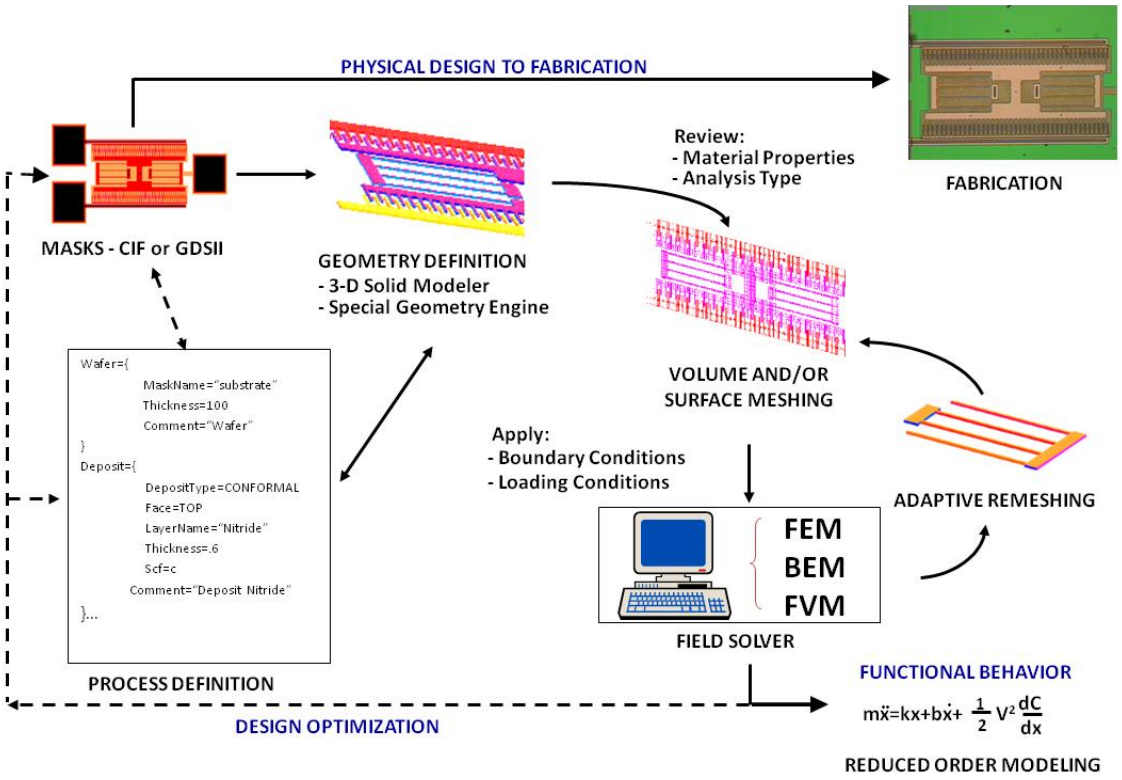


Figure 2: MEMS M&S design process

COMSOL can be applied to a variety of problems such as heat transfer, stress/strain analysis and modal analysis that can be solved using partial differential equation based methods like Finite Element Analysis (FEA). FEA is a numerical technique used to find an approximate solution to a given partial differential equation (PDE) with pertinent boundary conditions and parameters. Geometry is reduced into a discrete mesh of similar "elements", and properties and conditions are assigned likewise. Elements may be two-dimensional or three-dimensional. The process is computationally intensive as an increase in the number of elements for a given geometry increases the amount of calculations that are necessary to perform. Therefore, it is critical that care is to be taken to define the proper element mesh density to reduce computational resource consumption and solution time while obtaining reasonable results. Trade studies using FEA allow for the examination of output characteristics and modification of boundary conditions to meet desired performance goals. Solver adaptability is important in this step, as new technologies often require new governing equations and essentially new science. Some finite element solvers offer a fixed set of modes for analysis, i.e. structural, heat, etc., and lack the ability to adapt these solvers for new technologies. COMSOL software was created to address multiphysics problems so it is more adaptable to solving a variety of problems than some of its competitors. COMSOL's interface with MATLAB allows for customization of governing equations and model refinement with minimal manual manipulation.

Systems integration allows for the implementation of the physical device into an overall architecture for operation. Definition of the control circuits relevant to the individual device can be performed in the proposed process. Simulation Program with Integrated Circuit Emphasis (SPICE) software allows for circuit element definition and is compatible with select FEA programs. Iteration of analysis in both environments allows for refinement to achieve desired circuit characteristics and device performance. COMSOL has an integrated SPICE solver and provides the unique capability to integrate a finite element model with a SPICE model. Systems-modeling is shown as the final step in the M&S process shown in Figure 3 with the initial desire to utilize Very High Speed Integrated Circuit (VHSIC) Hardware Description Language (VHDL) software if possible. The ability to use VHDL would facilitate the integration of new alternative computing concepts with existing silicon-based computer technologies to create hybrid computing architectures. At this point very little effort has been spent on examining the ability to model alternative computing concepts in VHDL.

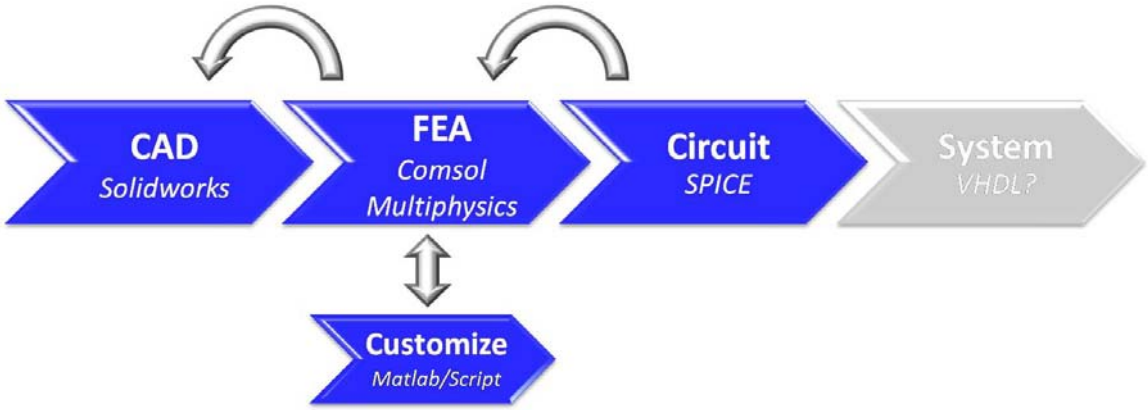


Figure 3: M&S process for hybrid computing architectures

3.0 NANOTECHNOLOGY

Numerous discussions and debates have occurred regarding the role of nanotechnology and how to define nanocomputing. Part of the problem is the hype associated with nanotechnology and the pursuit of new funding. People like to be part of the latest "hot" technology interest. This raises the question of whether or not the promise of the capability of nanotechnology is being oversold in order to get additional funds for existing R&D activity? Technology evolution is taking Complementary Metal Oxide on Silicon (CMOS)-based computing technology into the nanoscales. The fact that computer technology is being fabricated on a 45 nm line does not necessarily make it nanocomputing. If there is no new computing principle being exploited, then it is just that an issue of the size scale for classical computing technology getting smaller. Similarly, while the much smaller size may subject devices to quantum effects this also does not mean that one is doing quantum computing. All of this is based on the perspective that we are looking at alternative computing concepts for novel information processing paradigms that will provide revolutionary changes not evolutionary progression. By their very nature when biotechnology such as DNA computing and quantum information science such as quantum computing are finally realized they will most likely be implemented with nanotechnology, and thus could be considered examples of nanocomputing. Thus, for this project there was no major effort made to carve out a nanotechnology focus separate from biotechnology or quantum information sciences except for a quick look at carbon nanotubes.

3.1 General Thoughts

At the beginning of this effort some thought was given to as to whether or not existing M&S concepts are applicable to nanotechnology. There is a history of success at the Rome Research Site using a variety of M&S software to examine microelectronics and microelectromechanical systems (MEMS). Can this experience be brought to bear on nanotechnologies and other alternative computing concepts? The short answer is yes, but only after some effort has been made to understand the proper application of this experience.

In past work with finite element analysis, for instance, it was found for the particular software that was being used at the time, that if one kept the aspect ratio of the longest side to the shortest side of an element was equal to or less than 5 to 1 for a static analysis one could get very good results. In the case of conduction heat transfer it was found that one could use an aspect ratio of 10 to 1 with well formed elements. This understanding of the capabilities of this particular finite element software came as a result of years of experience and validation by several engineers. The pursuit of new technology to exploit for hybrid information systems requires the researchers to address multiphysics problems for which the rules of thumb for modeling and simulation are not broadly known. Different commercial vendors implement finite element analysis with their own biases and preferences necessitating the need to conduct trade studies to explore peculiarities of the software and understand how to utilize it properly. Some of these products may only address one type of problem well, but not others. Thus, one part of this project's effort was spent to look at how well commercially available software tools could be applied to the development of the technology for alternative computing concepts. For this project, SolidWorks for three-dimensional model construction and COMSOL Multiphysics for FEA were used.

During this quest for knowledge and understanding it was discovered that there are some "new" books available to help one begin to understand the issues related to the multiphysics modeling and simulation of MEMS and nanoelectromechancial systems (NEMS). [3, 4] It was also found that guidelines for the proper application of the Finite Element Method (FEM) for thermal and structural analysis are also available to the broader community. [5] This knowledge was previously limited to practitioners with years of experience behind them.

3.2 Carbon Nanotubes

Developers of advanced computing architectures constantly seek performance improvements in current devices while exploring the capabilities of novel concepts and the potential of new materials to provide superior properties, such as thermal transport, over existing material choices. As the sizes of devices continue to shrink, the density of these devices on a chip increases and in some case so does the heat generated. The correct thermal management scheme must then be employed to maintain the desired performance and reliability of systems. One of the benefits of having the proper M&S software tools is the ability to examine the potential of emerging materials and technologies, such as the Single Walled Carbon Nanotube (SWCNT), prior to any major investment in them. SWCNTs were examined to explore their potential for thermal management in future systems through the use of three-dimensional physical modeling.

3.2.1 SWCNT Background

SWCNTs are a focal point for researchers because of their high strength and exceptional transport properties. The SWCNT was "recently" discovered as a single sheet of graphite rolled into a tube. [6] The diameter of this tube is on the order of one nanometer (1 nm), while the aspect ratio of length to diameter can be greater than one thousand (1000x). [7] The orientation, also known as the chirality, of hexagonal units of the graphene determines whether the SWCNT is a metal or a semiconductor. [7,8] A Young's Modulus (E) on the order of 1 TPa has been experimentally demonstrated [7,9], supporting claims for its extreme stiffness and strength. As for the energy transport properties, a maximum current density of ~ 10^{10} A/cm^2 at a temperature of 250 ^{o}C [8] and a thermal conductivity demonstrated as high as 6600 W/m K [10] show promise for electronic applications. Table 1 below shows that SWCNTs appear to have superior thermal properties for heat transfer when compared to copper vias. [8] SWCNT supporters are quick to point out that, as copper interconnect technology shrinks down with the evolution of Very Large Scale Integration (VLSI) technology, issues with electro migration and excessive delay associated will be a concern. The resistivity of the copper interconnects increase as device size approaches the nanometer scale. Higher current densities could also lead to reliability issues when the capabilities of copper are exceeded. SWCNTs may provide an alternative to current technology to address the increase in heat generation and current density, eliminating the existence of electromigration and excessive delay.

Table 1. SWCNTs compared to copper vias

	SWCNT	Copper Via at the 22 nm node (expected year 2012)
Thermal conductivity (W/m K)	6600	400
Max Current Density (A/cm2)	~1x10^{10}	~1x10^{7}

There are a few issues with carbon nanotubes that must be resolved in order to take advantage of their potential benefits. Initial studies have shown that it is difficult to establish a solid contact to a single SWCNT, and therefore, the contact resistance is of significant concern. A proposed solution for this is to produce a bundled array of SWCNT as an interconnect. [8] This reduces contact resistance with a larger contact area while still exhibiting the material properties of interest. Another issue is that it is difficult to control the chirality of the SWCNTs in the bundle. [8] This means that there is uncertainty in the amount of conducting and semi-conducting SWCNTs which corresponds to unknown contributions to electrical properties. Other obstacles to carbon nanotubes come to light when the technology is looked at from the modeling and

simulation perspective. Material properties, specifically the thermal conductivity [10], lack a concrete definition with experimental values from different research groups ranging from several hundred to 6600 W/m K. Though most work has shown that it clearly is an excellent conductor of heat, uncertainty in the magnitude of the thermal conductivity yields difficulties in accurately quantifying this value when comparing theoretical models to experimental data. Finally, it is not yet clear if the SWCNTs may be modeled simply as a scaled continuum device, or if molecular mechanics need to be taken into account. [11] The Boltzmann Transport Equation has been used to model some devices on the nanoscale [11], however, it takes considerable knowledge to apply this concept. For this effort's brief look at SWCNTs, a simplified model will be used to obtain a general understanding of the characteristic response of SWCNTs with approximations and adjustments to classical theory.

3.2.2 Modeling Assumptions

To understand the application of carbon nanotubes for thermal management, a heat transfer model can be used. In general, there are three basic types of heat transfer: conduction, convection and radiation. Equations 1,2,3, and 4 below outline the three heat transfer modes and the corresponding contribution to overall heat transfer.

$$q_{cond} = -k\frac{dT}{dx} \qquad k = \text{thermal conductivity} \qquad (1)$$

$$q_{conv} = h(T_{surf} - T_{\infty}) \qquad h = \text{convection heat transfer coefficient} \qquad (2)$$

$$q_{rad} = \varepsilon\sigma(T_{surf}^{4} - T_{surround}^{4}) \qquad \varepsilon = \text{Emissivity} \qquad (3)$$

σ = Boltzmann's Constant (5.67×10^{-8} W/m^2 K^4)

$$q_{total} = q_{cond} + q_{conv} + q_{rad} \qquad (4)$$

In order to simplify the modeling of the heat transfer potential of SWCNTs, assumptions were made. First, one potential application of SWCNTs for heat transfer would be for electronics operating in a vacuum so convection was neglected. The contribution of radiation to the overall heat transfer was also considered very small and therefore could be ignored, leaving a heat transfer problem involving conduction. Another approximation for the modeling was to represent the carbon nanotube as a continuum cylinder with wall thickness of 0.34 nm. [12] Figure 4 below shows a diagram of the continuum cylinder with the attached reference frame coordinate axis.

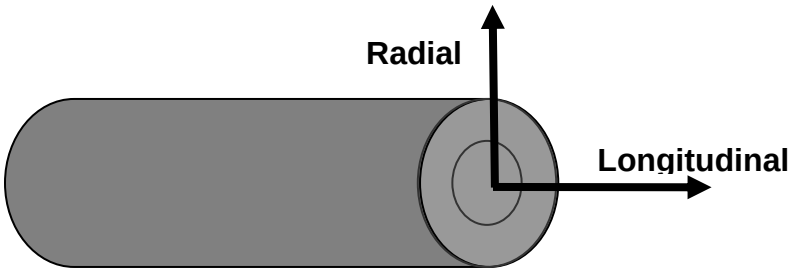


Figure 4: Continuum cylinder

Considering the significant aspect ratio of SWCNTs, the thermal conductivity has been shown to be anisotropic, meaning that the thermal conductivity in the longitudinal direction is considerably larger than the thermal conductivity in the radial direction. [12] An approximation within 5% for the anisotropic thermal conductivities of nanoscale objects has been documented in a fundamental heat transfer book. [13] This can be applied to carbon nanotubes, especially since the diameter is much smaller than the length. The approximation is based on the mean free path, or average distance traveled by an electron before it collides with either an imperfection in the material or with a phonon. This data is available from experiments, and all that is required for calculation is the bulk thermal conductivity for the material, or the material property of a macro-sized sample. Equations 5 and 6 below show the thermal conductivity approximations for the longitudinal and radial heat flow, respectively. All material properties were assumed to be taken at 300 K due to the lack of availability of experimental data outside of the room temperature range. Early results have also demonstrated a temperature-dependence [10] for the thermal conductivity of carbon nanotubes as well as a length-dependence, and with simplicity in mind, this can be ignored by keeping a constant cylinder length at a temperature of 300 K.

$$k_{longitudinal} = k_{bulk}\left[1 - \frac{\lambda}{3L}\right] \tag{5}$$

λ=electron/phonon mean free path

$$k_{radial} = k_{bulk}\left[1 - \frac{2\lambda}{3\pi L}\right] \tag{6}$$

The proposed heat transfer model adjusts the thermal conductivity to an anisotropic property in heat conduction for a SWCNT cylinder approximation. The following equation, Equation 7, highlights the model broken up into the radial and longitudinal components.

$$q_{Total} = -\left[k_{radial} \frac{dT}{drad} + k_{longitudinal} \frac{dT}{dlong} \right] \quad (7)$$

3.2.3 SWCNT Modeling in SolidWorks

There were two heat transfer modeling simulations used for SWCNT study. The first deals with a SWCNT connecting a silicon heat source and heat sink. This model was intended to demonstrate the difference in heat transfer capabilities for silicon and SWCNTs while highlighting the potential of a SWCNT to transfer heat efficiently from a source to sink. A 20 nm-long SWCNT with a diameter of 1 nm is connected to square blocks of silicon of dimensions 3 nm x 3 nm x 3 nm. The geometry for this model, created in SolidWorks, can be found in Figure 5 below. One issue of significance to modeling nanodevices, with the particular version of SolidWorks installed at the time, was encountered. SolidWorks had a seemingly arbitrary setting that would not allow any dimension to be entered that was less than 100 nm. This made it difficult to incorporate nanodevices with characteristic dimensions on the order of 1 nm. It was discovered, however, that a scaling procedure used in COMSOL during the importation of the model could compensate for this limitation and will be discussed later. The broader concern about this limitation is that that other analytical software programs will not be able to compensate for this anomaly.

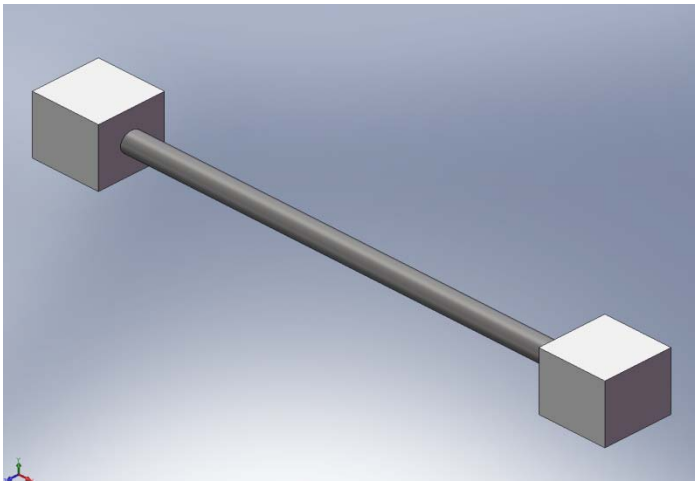


Figure 5: Initial SWCNT heat transfer model

The next model was meant to represent the three-dimensional stacking of chips in an VLSI electronics packaging concept in order to investigate the ability of SWCNT bundled interconnects to dissipate heat between layers. The model includes four 100 μm 100 x 1 μm silicon layers connected by bundles of SWCNTs with a plate of copper 50 μm x 50 μm x 1 μm on the top layer as a "source". The bundle "interconnects" are approximated as rectangular with a cross sectional area equal to that of a cylinder with a diameter of 1 μm and have a length of 5 μm. This approximation was done to make the importation of the SolidWorks model into COMSOL easier since the interconnects were considerably smaller than the other components in the assembly. This will be discussed in more detail in the COMSOL modeling portion to follow. Figure 6 below shows the three-dimensional stacking model as created in SolidWorks.

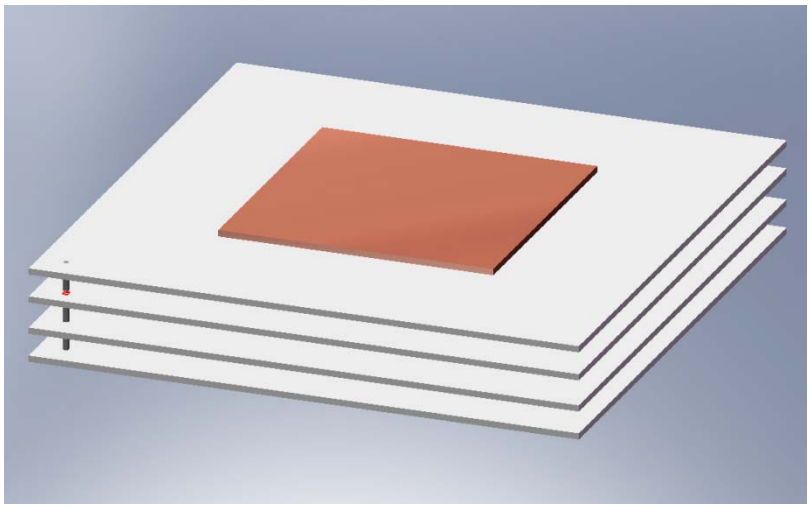


Figure 6: SolidWorks model of a stack

3.2.4 SWCNT Modeling in COMSOL Multiphysics 3.3

Two particular models are analyzed, as mentioned in the previous section. To import these models into COMSOL, special considerations were made due to issues with an arbitrary boundary of 100 nm in SolidWorks. The assemblies were created in SolidWorks at a scale of 1 nm = 1 m for the first model and 1 μm = 1 m for the second model, and this allows for a simple scaling of 10^{-9} and 10^{-6}, respectively, in COMSOL by use of the "Scaling" feature in the drawing application. This scaling was done in all three directions and this brings the component down to the characteristic size of interest. As stated previously, other analytical programs may not have this capability and therefore this feature must be taken into consideration during the geometry development in SolidWorks.

The first model uses the material properties from the bulk thermal conductivity of both silicon and SWCNTs. A thermal conductivity of 1.38 W/m K [13] and mean free path of 300 nm [8] are used for silicon. A thermal conductivity of 2000 W/m K [10] is used to illustrate an average of experimental and theoretical values in the range found by current researchers, while a mean free path of 1000 nm [8] is also used. These material properties are applied to the assembly at the sub domain level, which represents the entire volume of each component in the assembly. The anisotropic conditions as represented in Equations 5 and 6 are incorporated into the material properties by use of the "constants" function and according to the directional frame of reference. This allows for the adaptation of the modeling tool to solve problems on the nanoscale. The conduction problem is incorporated into the "General Heat Transfer" module in COMSOL by neglecting the convection and radiation components of the heat equation. The anisotropic conditions also modify the heat equation per Equation 7 and the temperature distribution is solved for once the appropriate mesh was generated. For boundary conditions, an arbitrary heat flux of 1.0e7 W/m^2 is applied to illustrate a realistic temperature distribution, with the magnitude per unit area being large due to the small cross sectional area at which it is applied. This value can easily be manipulated in an actual design model. Other boundary conditions include insulation where there is no heat transfer and an initial temperature of 300 K set at the trailing edge of the heat sink silicon block. This initial temperature provides a base point that can be analyzed after the heat flux is added for the solution.

A mesh was fitted to the geometry assembly sub domains to solve the heat transfer problem. One advantage found in the meshing application was the ability to mesh each sub domain separately. This allows for different mesh types to be applied to specific geometries. For this case, a triangular mesh is applied to the silicon block sub domains while a rectangular mesh was applied to the SWCNT with a triangular cross section. Some difficulty, however, can be experienced in this procedure. In Figure 7 below, a cross sectional view of the SWCNT cylinder is shown fitted with a triangular mesh. The issue with this is that a very fine resolution must be used in order to get the representative curvature of the cylinder. This becomes a computational problem since this creates a considerable amount of elements. COMSOL also does not allow for much variation from default mesh types for element size, shape, and resolution. The mesh can only be applied

uniformly to a component without control over concentration of elements in a single area. There is a necessity for a high resolution at critical points, especially at boundaries; however, the remainder of a large entity does not require as many elements. Figure 8 shows how the fine resolution is distributed in excess over the entire assembly. A user-defined mesh feature would be helpful in future versions of COMSOL, especially when models with a significant characteristic feature size difference are needed.

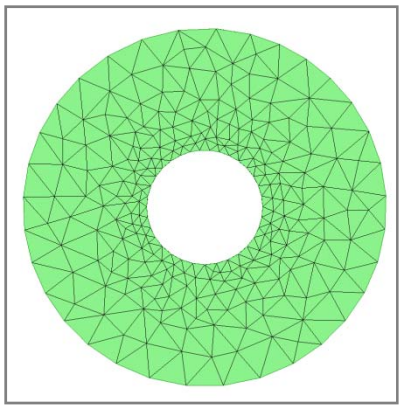


Figure 7: Cross sectional view of SWCNT model

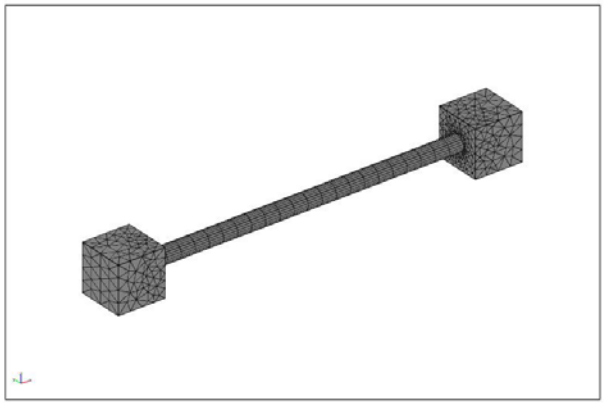


Figure 8: Initial SWCNT model fully meshed

After fitting the mesh, it is possible to solve the heat transfer problem in COMSOL for the geometry. Figure 9 below shows the resulting temperature distribution for the first model. It is evident in Figure 9 that the temperature distribution in the SWCNT is relatively constant. This can be viewed as illustrating the superior thermal conducting capabilities as compared to silicon since the heat is distributed more evenly throughout the SWCNT and there are no visible hot spots. Also, the anisotropic properties are apparent in the model since the temperature distribution is clearly only in the longitudinal direction and there is little variance in the radial direction for both the SWCNT and silicon.

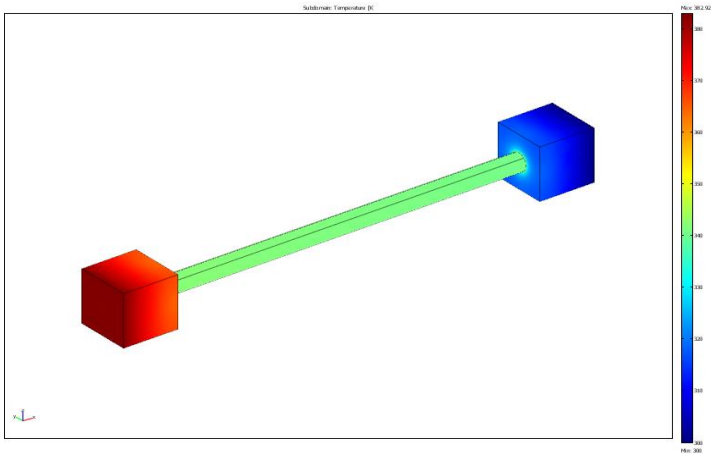


Figure 9. Thermal contours for initial SWCNT model

The second heat transfer model involves a more complicated assembly structure, and therefore, simplifications were made to analyze the model in COMSOL. A square array of SWCNTs was used to represent the interconnect as opposed to a cylinder to simplify the geometry. This simplification still provides the same effective area and theoretically, the same amount of heat flux for the problem while making it easier to generate the model and mesh. Properties used for the previous model are preserved for SWCNT interconnects and silicon in conjunction with anisotropic conditions for the components of small length scales. A bulk thermal conductivity of 400 W/m K [10] and mean free path of 40 nm were used for copper [8]. The scaling procedure was again performed to link the SolidWorks geometry with COMSOL. The arbitrary heat load of $1.0e^{7}$ W/m K was applied at the copper plate. The appropriate boundary conditions in areas of no heat flow were applied with a temperature of 300 K initialized at the bottom of the lowest silicon layer.

A mesh was applied to each sub domain to allow for some control of the element type. Problems associated with the previous model in meshing exist in this model. COMSOL, however, makes it possible to fit a dense mesh on the interconnects while fitting a coarse mesh to the other components. This is possible because the components are located in different sub domains. The smaller interconnects, which are the areas of interest, can have a finer concentration of elements, than the silicon and copper layers as shown in Figure 10 below.

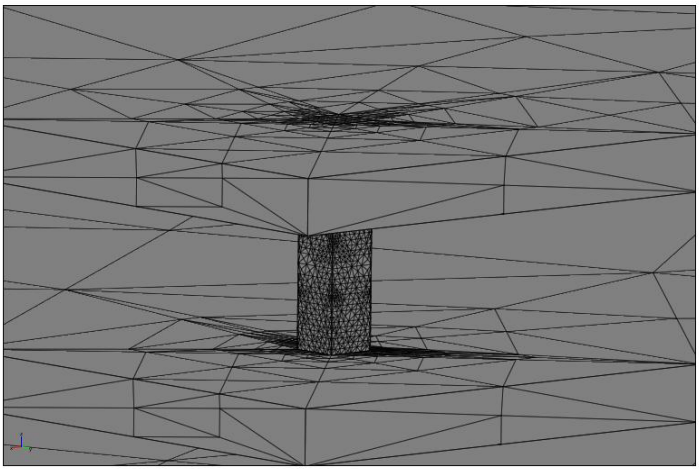


Figure 10: Illustration of the mesh variation for the different sub domains

After the mesh generation was completed, and the appropriate load and boundary conditions applied, COMSOL could solve the heat transfer problem. Figure 11 below shows the resulting temperature distribution for the stacked model. The results illustrate the largest temperature difference being between the layers, with the lowest layer remaining at the coldest temperature. Figure 12 is a close-up view of a SWCNT bundle interconnect in the three dimensional stacked model. The results are consistent with the previous model in that the temperature distribution is relatively constant through the bundles.

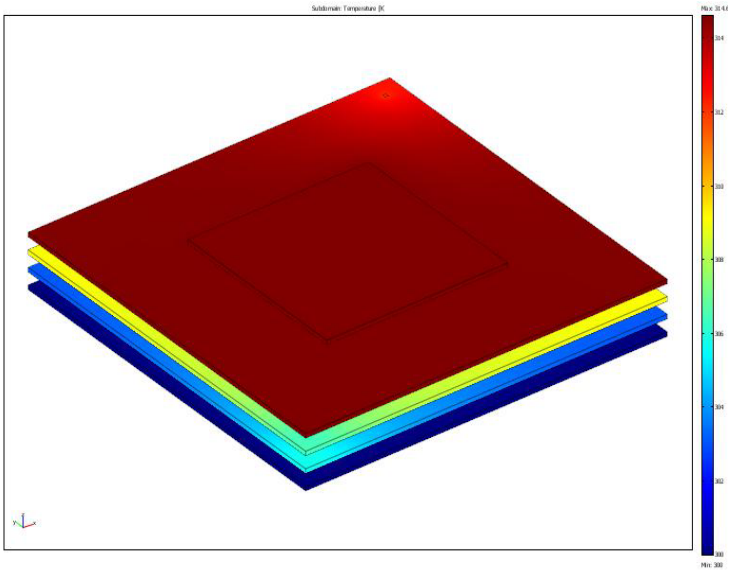


Figure 11: Thermal contours for stacked model

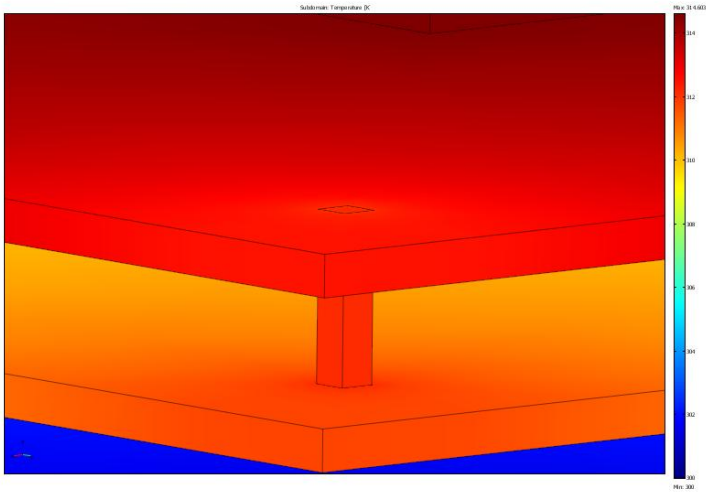


Figure 12: Close up of interconnect interface with larger layers

3.2.5 SWCNT Concluding Remarks

In the examination of SWCNTs assumptions were made to facilitate heat transfer modeling trade studies of this technology. These simplifications when done correctly during model creation permit the use of existing commercial software packages in the exploration of the applicability of new technology. The results from this portion of the effort suggest that SWCNTs might be beneficial for future computing technology. Three gaps in technology stood out in this portion of the project. First, a solid understanding of the characteristic material properties of carbon nanotubes appears to be missing. Second, additional work is needed to understand the role of molecular effects in heat transfer modeling of nanodevices. Third, users of commercial software packages need to be aware of potential limitations in a particular packages ability to model the feature sizes of the nanodevices of interest.

4.0 BIOTECHNOLOGY

Biotechnology opens the door to several different approaches to not only alternative computing concepts, but also alternative means of fabrication. There are many ways to view biotechnology and to help categorize the various research areas the following definitions, defined in a previous project [2], are used:

a. Biomolecular Computing is computing with biological material.
b. Bio-inspired computing is the mimicking of biological processes on silicon.
c. Bioinformatics is, "an interdisciplinary field bringing together biology, computer science, mathematics, statistics, and information theory to analyze biological data for interpretation and prediction."[14] Basically, this involves the application of computer science to process data for medical and biological research.
d. Biocomputing is the broad term that covers the pursuit of computing technology which encompasses biomolecular computing, bio-inspired computing, and bioinformatics.

The original intent of looking at this area of alternative computing concepts was to further explore how one would conduct the proper modeling and simulation process for designing and building a biomolecular computer. This portion of the project, however, changed directions a few times as a result of becoming wiser about the limitation of some concepts along with an organizational change and the resulting change in technical direction for the CTC and support for this area of research. M&S work in the area Biomolecular Computing, for instance, never materialized as envisioned. This section of the report will provide a quick snapshot of what was done, an area of interest to watch and an introduction to the current area of activity.

4.1 Membrane Computing

Membrane Computing, also known as P-Systems, is relatively new concept, coming into existence in 1998 when Gheorghe Paun published his first paper on the subject. "Membrane Computing is a bio-inspired branch of natural computing, abstracting computing models from the structure and functioning of living cells and from the organization of cells in tissues or other high order structures." [15] This concept was initially looked at for two reasons. First, could computational biology tools such as those found in the Bio-SPICE environment be used to model a membrane computing function? It was quickly determined that the available systems biology tools were not appropriate for modeling P-Systems. Second, there was some research that indicated that there was a little interest in a hardware implementation of P-Systems [16], at the time this area was examined for this project it did not seem too promising. Thus, it seems like the role for P-Systems is more along the nature of software or algorithm development. Since this effort is focused on examining how alternative computing concepts could be implemented in hardware no further research in this area was pursued. If the reader is interested in learning more about P-Systems, a good starting place for further reading is at: http://ppage.psystems.eu/.

4.2 DNA Self-assembly

Part of the problem with the biomolecular computing area was that research and development activity in other organizations seems to get diverted from pure information technology related applications into medical applications. This diversion is a barrier to the sound development of clear path forward for the broad community for biomolecular computing. It is hard to maintain local support for a technology area when there is not a larger community asking it. One area in biotechnology that has some potential and will need to be watched is the area of DNA self-assembly. Simply stated, this is the use of synthetic DNA to fabricate nanoelectronics. Interest in this area comes from the debate of Moore's Law, and whether or not existing lithographic processes, currently used in electronics fabrication lines, can be refined to be applicable for the small size scales of future electronic technologies. Researchers feel that the use of DNA self-assembly may provide an alternative approach for nanoelectronic fabrication. There are numerous sources on the internet for which readers interested in learning more about this area. The book, "Introduction to DNA Self-Assembled Computer Design," by Professors Christopher Dwyer and Alvin Lebeck at Duke University is another resource from which one could learn more about this area and how it could apply to computer design. [17]

4.3 Structural DNA Nanotechnology

This aspect of the project seeks to establish the foundation for utilizing structural DNA nanotechnology in future Air Force systems. Current activity is focused on enhanced situational awareness through advanced taggant design. The desire is to leverage past work with computational design tools and DNA to capture the fundamentals for the design of optimized, complex, covert molecular taggants utilizing structural DNA nanotechnology. Future reports will provide more details on this research area.

5.0 QUANTUM SCIENCES

Quantum computation is a novel paradigm of information processing that may provide significant advantages over classical computing methods allowing one to solve profound problems that are otherwise unattainable, such as the ability to factor large numbers. [1, 18] The physical implementation of quantum computing architectures will require novel technology and methods that are not easily supported by current design tools. Therefore the objective of this portion of the project is to explore what is needed for a proper M&S environment by examining the flexibility and adaptability of commercial tools.

5.1 Nanomechanical Resonators

One approach to the practical development of a quantum computer involves the use of nanomechanical resonators. Nanometer-scale, resonating beams are being explored as a possible avenue to exhibit quantum behavior such as superposition and decoherence. [19-21] Numerous research efforts are being conducted to simulate the behavior of these nanomechanical devices in order to understand how they can be designed, modeled, and applied to quantum computing. This potential development of quantum computers utilizing nanomechanical based processors relies on achieving an accurate model of the mechanical system. An interesting aspect of this portion of the project is that, over its duration, new versions of the SolidWorks and COMSOL Multphysics software were installed. Comparisons of selected features will be made below.

5.1.1 Initial Assumptions and Constraints

To develop a model that accurately depicts the behavior of a nanoscale resonating beam, several factors related to building the proper model needed to be examined. In the literature review that was conducted, it was discovered that current nanoscale models ignore molecular details. [22] The object and components of the system are modeled as a continuum, allowing classical mechanics to be used to model a simple beam. Also, experiments have shown that density, temperature, velocity and displacement can be assumed as being smoothly varying. This means that there are no drastic rate-of-change anomalies, or “jumps” in any of these values when a variable is introduced into the system.

Next, body forces are ineffective at deforming structures compared to surface forces on the nanoscale. This is simply a scaling observation and means that the weight force due to gravity is so small with respect to any load force, i.e. an electrical driving force (applied voltage), that it can be considered negligible in that it will not affect the distance the load force will bend the device in the direction of the gravitational weight force.

Material properties are another important aspect of assumed conditions on the nanoscale level. Currently, researchers and scientists are using the same values that have been determined experimentally [23] on the microscale level. [24] However, these material properties assumptions leave out the temperature dependence of the material properties. All experiments have been run at cryogenic temperatures at or around zero Kelvin, which

does not allow for a variance in temperature and therefore provides no insight as to how the properties may change during heating or cooling. Since material properties change from the mesoscale to the microscale, it is also expected that they change from the microscale to the nanoscale. This paradox, however, has not been addressed with much detail yet.

Along with the aforementioned assumptions there exist constraints that are imperative in modeling a nanomechanical beam. A maximum voltage boundary exists on the system. Since an electrostatic voltage signal is used to drive the system into resonance, it is important to determine how much voltage can be applied. This maximum voltage value is known as the "snap-in", or "collapse" voltage because if the voltage exceeds this value, the resonator risks collapsing onto the substrate permanently, disabling the device. [25] A modification must also be made to the simple harmonic motion, or "mass-spring" equation, in order to accurately model a nanoscale device. The fundamental mass-spring equation is shown below. [26] Constants "m", "c", and "k", represent the mass, damping constant and spring constant, respectively. The Term "x" refers to the displacement, while "v" and "a" refer to the velocity and acceleration, respectively.

$$ma + cv + kx = 0 \tag{8}$$

This equation implies that velocity approaches zero over time. Then, since temperature is a measure of motion of molecules and therefore is proportional to the velocity of the molecules, this would imply that the temperature would also approach zero. Since this model is on the nanoscale, and the nanoscale deals with objects at or above molecular size, temperature is directly proportional to velocity. With that, if the device stops oscillating and moving, then temperature would have to be zero. However, this violates the 2nd Law of Thermodynamics where the temperature of a system cannot vary from the temperature of its surroundings. [26] Therefore, a new motion equation that includes a driving function to keep the system in equilibrium is necessary. [26] This equation is shown below:

$$ma + cv + kx = f_n(t) \tag{9}$$

5.1.2 Mechanical Model

In order to understand the characteristics of a nanomechanical system, it was necessary to generate a simple mechanical model. The aforementioned assumptions need to be applied in this aspect of modeling. To simulate a nanostructure that resonates and is fixed at both ends, a simple beam was chosen as the basis for the model. The beam is fixed at both ends and has length L and cross sectional dimensions w and t, as shown in Figure 13.

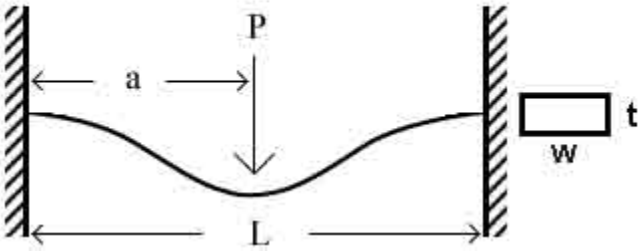


Figure 13: Illustration of basic beam

This simple model allows for the calculation of the resonance frequency, as well as the deflection under an applied load. Figure 14 below shows the coordinate reference system used, as well as the pertinent geometrical parameters for the model.

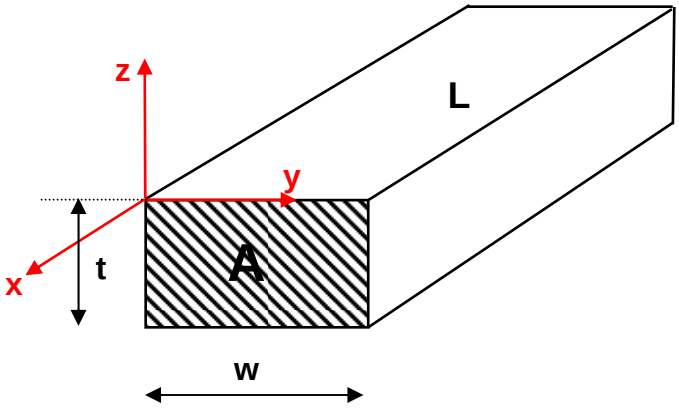


Figure 14: Coordinate reference system for beam

The deflection in a fixed-fixed beam can be calculated using classical mechanics. The ends are assumed to be fixed, but free to rotate, which eliminates any torque or moment on the beam. The characteristic equation for the deflection of a fixed-fixed end beam of this sort is readily available in mechanics of materials books [27] and is shown below:

$$\delta = \frac{PL^3}{48EI} \tag{10}$$

Parameters present in the deflection equation that have yet to be defined include the load, P, E, and the moment of inertia, I. The load is a value that is defined by the applied voltage which is not the focus of this analysis. Young's Modulus is a material constant and can be obtained from experimental values that have been discovered and implemented in other micro and nanoscaled system modeling. [23, 24] There is some concern, however, that the current material property assumptions do not apply on the nanoscale. The moment of inertia is a source for confusion in modeling any mechanical system. In order to accurately portray the moment of inertia in this equation, the direction of oscillation needs to be determined. In this model, the beam oscillates in the z-direction (refer to diagram above). With this, the beam oscillates around the y-axis and therefore the moment of inertia is taken about the y-axis. [28] The characteristic equation for the moment of inertia about the y-axis [27] for this model is shown below:

$$I_y = \frac{1}{12} t w^3 \tag{11}$$

The resonance frequency can also be modeled and is quite useful in a nanomechanical resonator. By knowing the resonance frequency, measurements of frequency can be used to tune the device to sense electronic signals in the beam or changes in frequency. [29] To model the natural frequency, the fundamental equation shown below is used:

$$f_n = \frac{1}{2\pi} \sqrt{\frac{k}{m}} \tag{12}$$

A more useful version of this equation incorporates the fundamental resonance mode (the first mode) into the equation yielding the natural frequency. [26]

$$f_n = 1.03 \frac{t}{L^2} \sqrt{\frac{E}{\rho}} \tag{13}$$

Parameters for this model include geometrical as well as material properties. The geometrical properties are outlined in the model, as well as E. The density, ρ, is another material property that has to be obtained by dividing the mass by the volume of the object.

5.1.3 CAD Drawing and Analysis

The first step was to develop a geometrical model. Figure 15 shows a screenshot of the nanomechanical resonator beam assembly created in SolidWorks 2005 based on dimensions from documented work [30] and material properties from experimental results. [23] It consists of a gold layer 60 nm thick and a silicon layer 185 nm thick. It is 10.7 μm long, and each finger extends 400 nm off of the base section. The ability to include material properties in the three-dimensional model is extremely useful in finding the mechanical characteristics of the structure. This capability also allows the user to determine section properties from the geometry of a model. For example, the required moment of inertia around the y-axis can be determined in the section properties solver, which again pertains to a required parameter in the resonating beam model.

The only difficulty encountered in this model in the SolidWorks 2005 software was the unit limitations. The program is capable of calculating values by utilizing scientific notation and even allows for the assignment of user-chosen units. For example, nanometers were used in this model because they best described the geometry. A size limitation exists, however, in many of the feature tools. In an extrude feature, 100 nm is the smallest value that is allowed for creating a solid. This was a major setback because the 60 nm gold layer is obviously less than 100 nm thick. This did not appear to be an issue with solving for the geometry, but an arbitrary limit set by program developers. This obstacle was overcome by extruding the feature 160 nm, then cut-extruding the feature by 100 nm, leaving 60 nm of material as a solid.

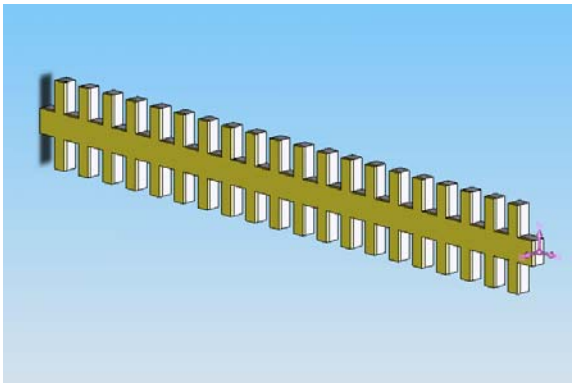


Figure 15: Initial SolidWorks model of nanomechanical beam

5.1.4 Finite Element Modeling and Analysis

Finite Element Analysis, or FEA, is an essential process in mechanical design and modeling in that it looks at the physical properties and characteristics of a system under loading and/or transient conditions. Comsol Multiphysics 3.2 is an FEA program that has the ability to produce system models from established geometry, loading conditions and constraints. The "Static Analysis" feature allows for the modeling of deflection of a simple beam under loading conditions. The "Eigenfrequency Analysis" offers an avenue to calculate the resonance frequencies under different modes. These two features of the program are pertinent to the nanomechanical resonator model because deflection can be modeled under a certain electrostatic load from an applied voltage, and the resonance frequency can be determined. Stresses and deflections can be determined for the nano beam at resonance. This simulates the device oscillating at high frequencies close to resonance. The modeling software can not only calculate values, but also generate plots and animations of a given model.

One last feature of the software is its "Import CAD" feature. This feature allowed geometry files created in SolidWorks 2005 to be incorporated into geometrical objects in the COMSOL window. This feature was useful because it saved a significant amount of drawing time in COMSOL and allowed for accurate geometry to be portrayed and analyzed. A few difficulties were encountered, however, while importing assembly files from the SolidWorks package into COMSOL. It was later discovered, after a correspondence with a COMSOL Technical Representative, that the current version, version 3.2, does not support assembly files automatically. [31] This means that the program was unable to model assembly files completely as imported from SolidWorks since the transition between CAD files and FEA geometry is not smooth, causing some geometry characteristics to be lost. [31] There were a few possible solutions to this issue. First, a full geometry file could be created using separate geometry files. Basically, this would assign geometrical reference points to two different objects, and where they interact, these reference points would be the same. However, this task proved to be tedious and time-consuming. The second approach involves generating a MATLAB file to construct the geometry with an ".m-file" script. This method could be valuable if modified to allow for user inputs. This would allow easy rebuilding or would allow iterations with different geometry to test the effects of changes on the system and its characteristics. However, the code approach is difficult to implement for novice programmers and therefore was not pursued. The last alternative was to construct a hybrid structure that contained the same geometry as the assembly and only varied in material simulation. Instead of having two materials, this structure would have only one but it would be an effective material. The only value that varies and does not agree with the assembly is E for the two materials. An effective E may be obtained in this application from the following proportion of volumes of the two materials.

$$E_{eff} = \frac{E_{gold}V_{gold} + E_{silicon}V_{silicon}}{V_{total}} \tag{14}$$

With this effective E it was possible to run the modeling analysis. The Eigenfrequency analysis result yielded a resonance frequency similar to that calculated by hand, proving the validity of the Finite Element code. Also, the deflection could be modeled under this resonance mode and the stress could be calculated as well. Figure 16 below shows the stress model for the first mode resonance frequency in Eigenfrequency analysis:

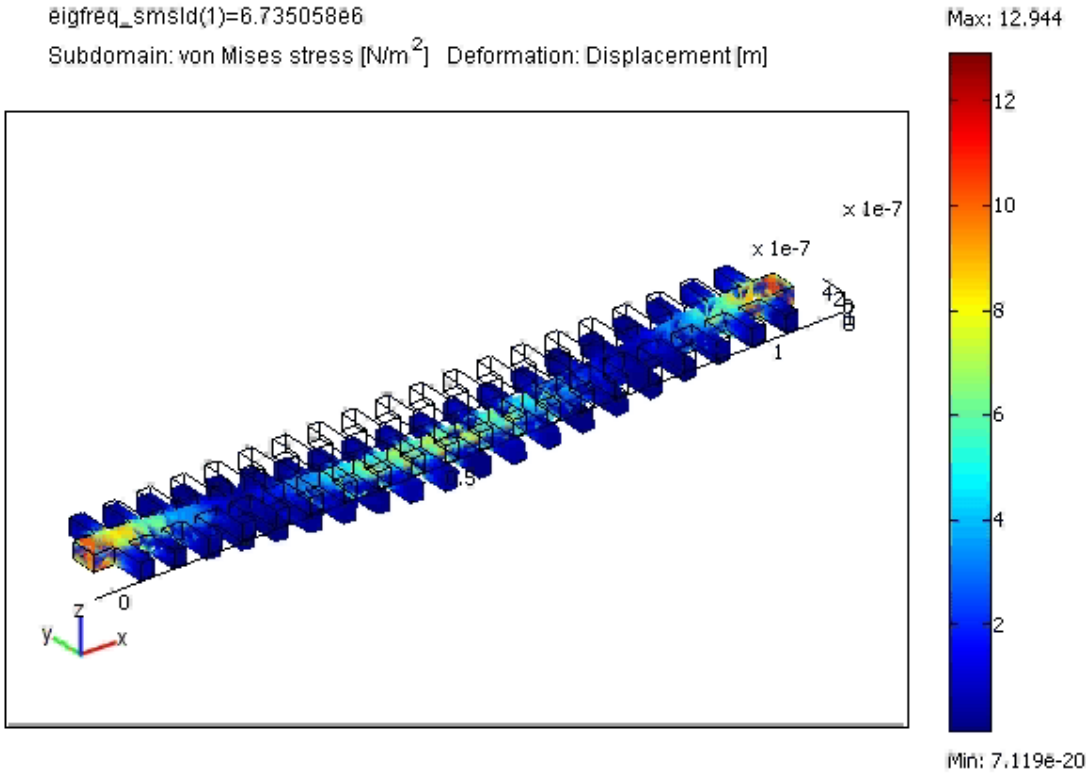


Figure 16: First mode response for beam

As is seen in the above graphic outlining the stress, the Eigenfrequency output "eigfreq_smsld(1)" corresponds to the first mode resonance frequency and is given as 6.735×10^6 Hz. The maximum stress experienced is located at the ends and is shown in red. The typical shape of the first mode resonance frequency is experienced in this model with the one peak oscillating up and down. This analysis tool proved helpful in understanding the characteristics of a nanostructure beam.

COMSOL Multiphysics Version 3.3 brought with it a significant improvement in the capabilities of its troublesome import feature discussed above. Version 3.3 was able to handle complex structures with multi-layered geometries. The improvement of the "Create Composite Object" feature eliminates redundant interior boundaries while still recognizing different components and allowing for characteristic material properties to be applied. Figure 17 highlights the assignment of material properties to the different component sub domains created in SolidWorks and imported in COMSOL.

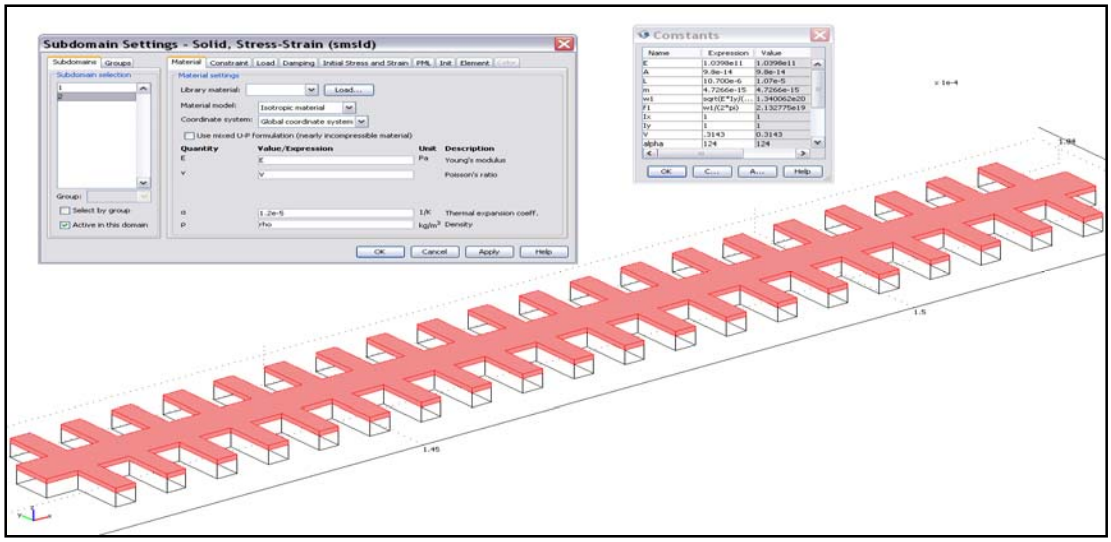


Figure 17: Snapshot of sub domain material definition for beam geometry

Simulations were rerun under COMSOL Version 3.3. Figure 18 below shows the third mode Eigenfrequency response of the beam in COMSOL. The magnitude of the frequency and the mode shape were both shown to have good agreement with the documented results from researchers at Boston University. [30]

5.1.5 Nanomechanical Resonator Concluding Remarks

An introduction to the fundamental details and complexity of modeling a nanomechanical resonator has been provided. Through a literature review it was discovered that little research has been conducted on nanomaterials under both room temperature and cryogenic conditions. A better understanding of material properties on the nanoscale and their impact on quantum mechanical modeling will be needed for future research in order to more accurately model nanodevices and systems. Commercially available software proved to be a very useful in modeling a nanomechanical resonator beam.

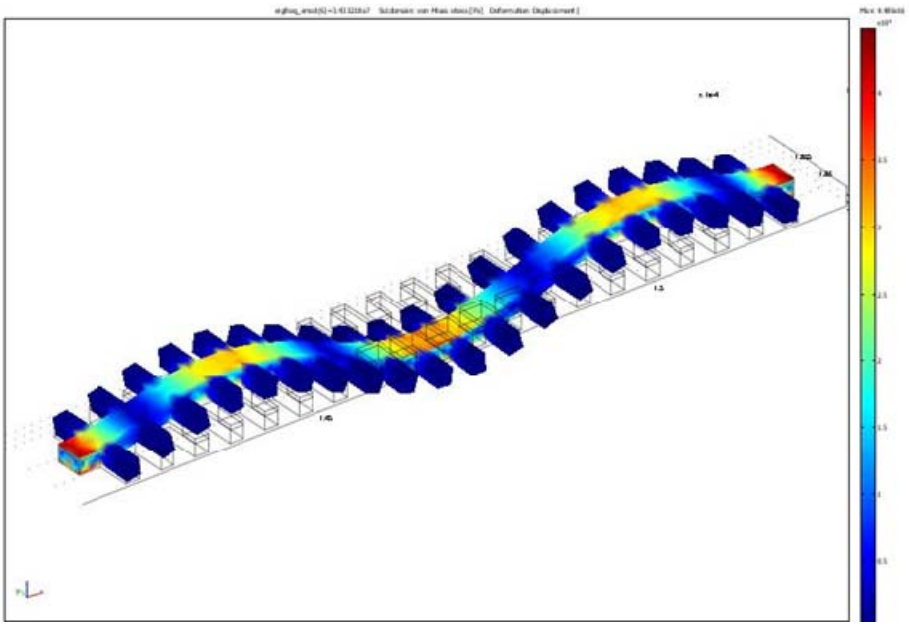


Figure 18: Third mode response for beam

5.2 Ion Trap

A second approach to quantum computing being pursued by some researchers is the use of ion traps. Basically, ion traps encode and process data with a string of ions that are confined in a field. The field depends on the type of ion trap: the Penning Trap makes use of magnetic fields, and the Paul Trap, or Linear Trap, utilizes radio frequency (RF) electric fields. Lasers are used for inputs, as well as a means of laser cooling ions. [32] The promise of the ion trap lies in its basis on relatively well-known technology. Fabrication of the proper device geometry for ion trap concepts can leverage a combination of MEMS, CMOS [33] and Gallium Arsenide (GaAs) [33, 34] technology. At the forefront of research into ion traps is a group at the University of Maryland, led by Christopher Monroe (previously at The University of Michigan). [34, 35] Investigation into planar geometry of ion traps by the Maryland group has led to an understanding of the hyperbolic electrode model, as well as the influence of geometrical relationships and aspect ratios on the potential field. [34] They have also developed a concept for a scalable array of ion traps, thus adding more merit to the ion trap becoming a practical means of building a quantum computer. Another group from Imperial College of London has focused on the scalability of ion trap chip design and its implementation with existing fabrication technology, specifically by using of existing silicon-based MEMS processes. The Imperial College group reaffirmed the importance of geometry and aspect ratio on the efficiency of the device, as well as proposed the consideration of resonance frequency and RF heating as modeling parameters. [33] Published models and research by these groups provided a basis for investigation of the applicability of commercially available M&S software for the design and analysis of ion traps. The pertinent parameters that are to be investigated include the electric field for ion confinement [32-34] and the resonance frequency for mechanical validity. [33] This portion of the project also provided insight into the idiosyncrasies of modeling ion traps.

5.2.1 Ion Trap Model Generation

Ion trap geometry was implemented into SolidWorks according to the existing Imperial College design. [33] The structure consists of, essentially, five layers: a silicon base, two silicon dioxide surrounding layers, and two gold electrode layers. Reducing the structure into components of each layer in an assembly allowed for different material assignment with correct geometric relationships. Embedded properties and appearance for the prescribed materials allowed accuracy in representation and visualization. Figure 19 shows the completed geometry structure from SolidWorks.

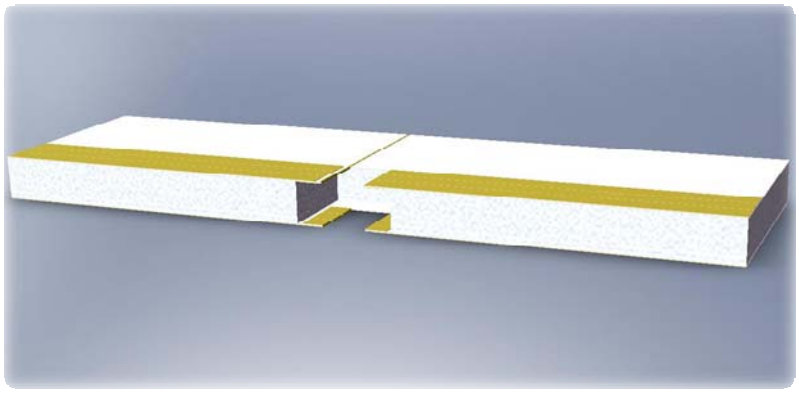


Figure 19: CAD model of individual linear ion trap

5.2.2 Ion Trap Analysis

The initial work with ion traps was interested in the resonance frequency, a mechanical parameter, and the electric field, an electronic phenomenon. COMSOL possesses a built-in geometry generator, which is beneficial for reducing complex CAD models to offer a reduction in model size and ultimately solution time. This feature, along with the MATLAB interface, means that the iterative nature of the modeling and simulation process does not imply starting over from scratch. Previous modeling work can be recycled and reused.

The resonance frequency of the ion trap structure, specifically the electrodes, must be sufficiently far from the RF input frequency to avoid interference. [33] Therefore, it is necessary to investigate the resonance frequency of the electrodes and structure to ensure there will not be interference. A simple approximation of the geometry is found in Equation 15 below for the electrode from the ion trap with length, h, and width, w, modeled as a cantilever. The approximation neglects the gold electrode layer and only uses silicon dioxide and its relevant material properties in Equation 15. With the published dimensions from the design [33], a frequency of 154 kHz from this model was found to be sufficiently far from the drive frequency of about 21 MHz.

$$f = 2\pi\left(0.16\sqrt{\frac{E}{\rho}\frac{w}{h^2}}\right) \tag{15}$$

To validate this approximation, FEA was performed on the simple structure of exact dimensions and material properties. Agreement was found within 1 percent, adding confidence in modeling procedures as well as the software package. To add a more realistic approach to the model, the gold layer for the electrode was introduced using the prescribed process. A solution of approximately 96 kHz can be found in Figure 20 below. This result was considered reasonable, as adding mass reduces the frequency

according to Equation 15. A simple hand calculation of the more complex geometry of this structure, however, was not possible. The number of elements required to obtain a solution was also investigated in this portion of the project. This work established an understanding of the complexity necessary to achieve a certain level of accuracy, providing insight to simplifying complex models for future work. Mesh refinement was inputted manually and the solution and convergence time were recorded for each case. Figure 21 shows the result for the mesh case study. Clearly, solution time increases significantly as mesh refinement increases. However, the accuracy of the solution was not affected by more than 5 percent. This suggests that in future modeling, mesh refinement may be coarse for complex models to still achieve a reasonable degree of accuracy. This will save significant resources, allow for reduction in time to optimize geometry and integrate analytical results into system models.

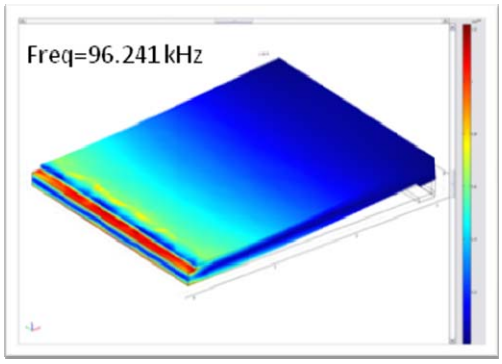


Figure 20: COMSOL resonance frequency of electrode

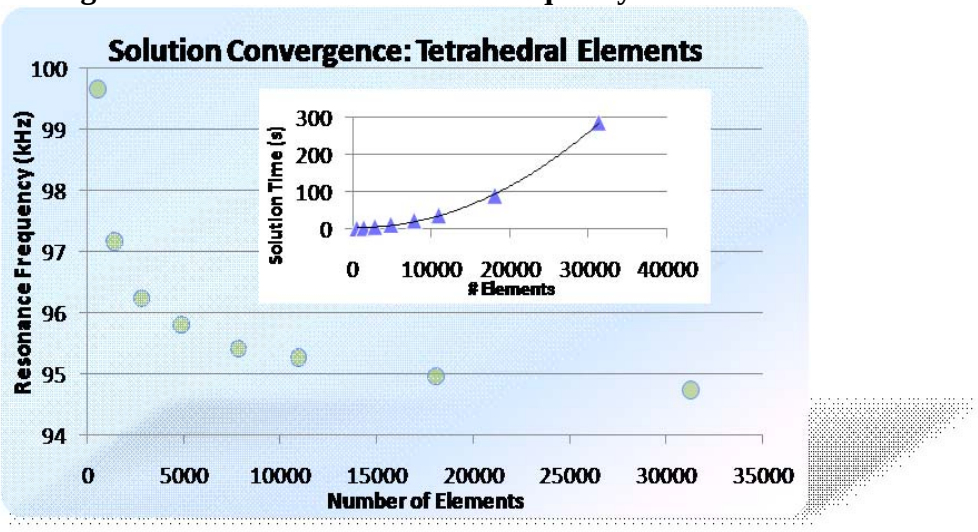


Figure 21: Mesh case study results

The knowledge gained from the case study was applied to the entire geometry structure. Figure 22 shows the geometry mesh case for the ion trap zone and Figure 23 shows the results of the analysis. A solution of about 93 kHz is approximately 3 percent different than the simplified case. The significance of this correlation of results is that it provides an option to performing several small, simplified studies with individual models when a single model can be reused several times.

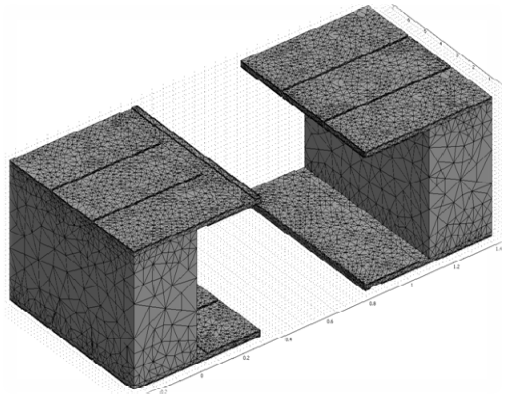


Figure 22: Mesh structure for resonance frequency

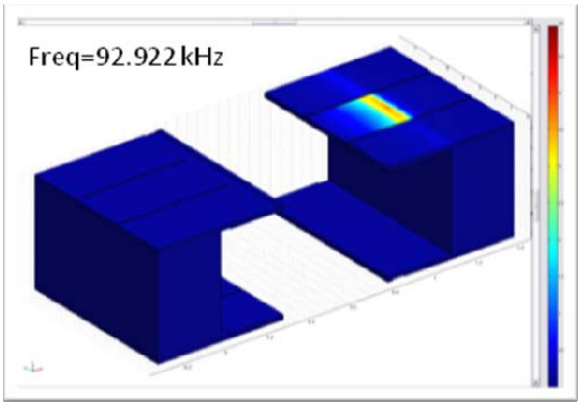


Figure 23: Solution for resonance frequency

The electrical characteristics were also pertinent to our performance output goals of the modeling and simulation process. A stable trapping potential must be maintained to confine ions. [33]

The RF drive voltage, $V_o \cos \Omega_T t$, and DC endcap voltage, V_{dc}, are constant parameters in the model, while the voltages V_{c1} and V_{c2} are variables that adjust the electric potential field. In modeling the field in the simulation process, these variables can be adjusted to obtain the desired trapping potential. COMSOL and its AC/DC module were used to investigate this model with time-harmonic boundary conditions according to the RF input. For the RF voltage, there must be an outer boundary condition that defines the perimeter. Elements must also be present in the zone (as opposed to open space) in order to have a solution in that zone. Therefore, the ion trap zone structure was enclosed in a box, as was shown in the top of Figure 24, allowing for the definition of the boundaries as well as a medium between electrodes to solve for the potential field. The drawback to this approach, however, is the complexity of the model and the issues encountered with aspect ratio errors. According to the electrode geometry, the outer box is many times larger and thus requires hundreds of thousands of elements to obtain a result. This is not practical, as the solution time is significant. With this, the geometry generation capability of COMSOL allows for modification of the CAD structure to only include the trap zone. Figure 24 illustrates this transformation and shows the reasonable mesh incorporated into the structure. Application of the boundary conditions allows for solving of this structure, and the solution may be found in Figures 25 and 26.

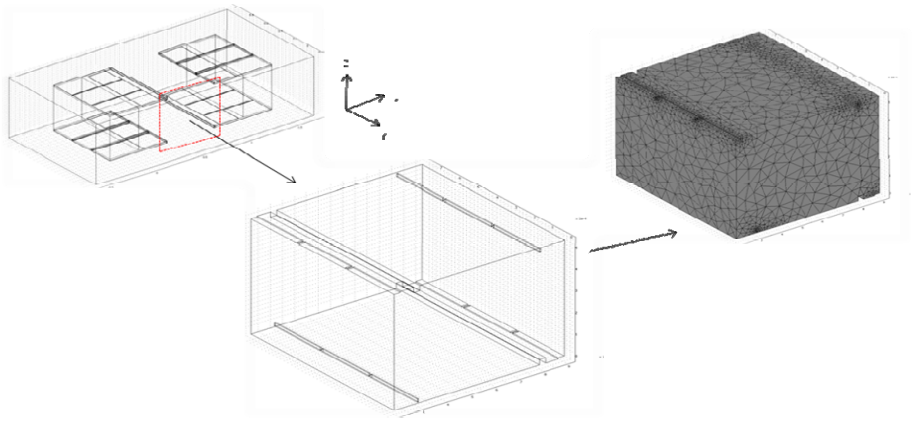


Figure 24: Simplification of ion trap geometry for solution

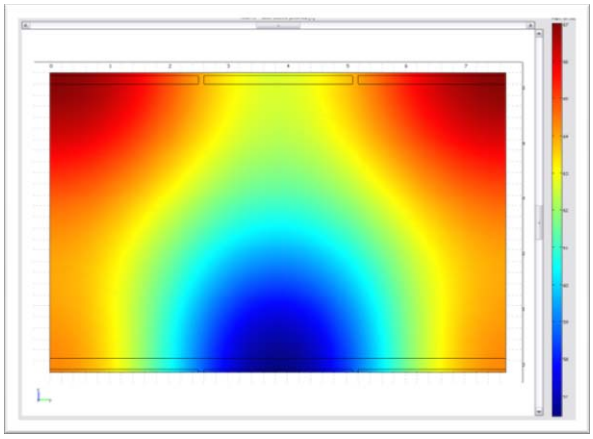


Figure 25: View of potential field in YZ plane

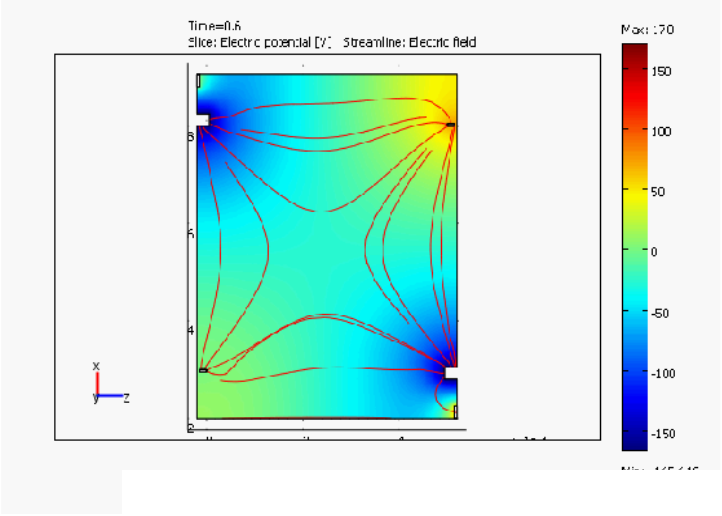
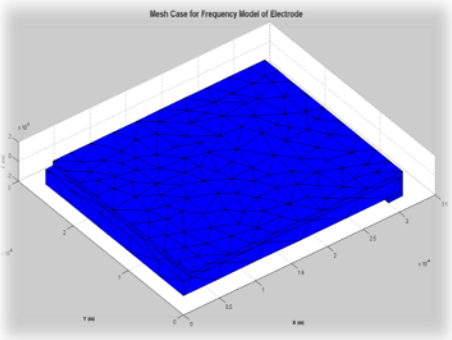


Figure 26: View of solution in XZ plane

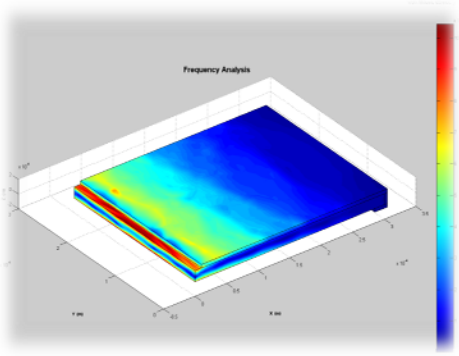
The solution illustrates a hyperbolic electrode geometry similar to and in good agreement with that documented by the University of Maryland group. Modification and refinement of electric potentials V_{c1} and V_{c2} allows for fine-tuning of the trap zone to achieve the desired field. The FEA package in COMSOL Multiphysics allows designers to perform case studies which, though tedious, offer suggestions on the implementation of the entire model.

5.2.3 Scripting and Customization

To allow for more flexibility in models, especially those not supported by COMSOL Multiphysics or other FEA packages, scripting and code generation are necessary elements of the design process hierarchy. COMSOL, as was previously mentioned, included a MATLAB [36] interface as well as its own, stand-alone scripting program. [37] With this, you are able to save models as ".m" extensions to convert to MATLAB format. This allows for integration of any MATLAB function, as well as use of existing COMSOL functions simultaneously running in MATLAB. Another helpful feature is the ability to use the MATLAB command window to execute or research (via help) COMSOL commands. This is applied in debugging, as well as in verifying the status of the solution. A significant benefit of the MATLAB interface is found in the ability to incorporate any mathematical relationship, such as a novel and thus unsupported governing equation, into the COMSOL model. This includes writing programs to use looping to perform a case study. An example of the application of a program loop can be found in the analysis of mesh refinement from Figure 21. Recall that manual input of mesh refinement was necessary, as well as manual recording of the pertinent output values. This tedious process can be eliminated by writing a script to perform the analysis with different mesh cases while recording the solution and plotting. By converting the initial model file from the resonance frequency to a MATLAB ".m" file, the boundary conditions and geometry are all preserved and all that is necessary is to modify the code to incorporate the loop. The output parameters are solved for and recalled from the COMSOL functions in MATLAB, and recorded for post processing. Figure 27 below shows a result of an iteration of the case study which is similar to that of Figure 20.



Mesh Performed in Matlab



Solution Computed in Matlab

Figure 27: Response frequency solution from MATLAB

The results in Figure 28 demonstrate a plot similar with similar trend to that in Figure 21. It is evident that the solutions are not exactly the same as those found in COMSOL, and this is due to the difference in solving algorithms between the two programs. However, the overall solution accuracy is within 1 percent.

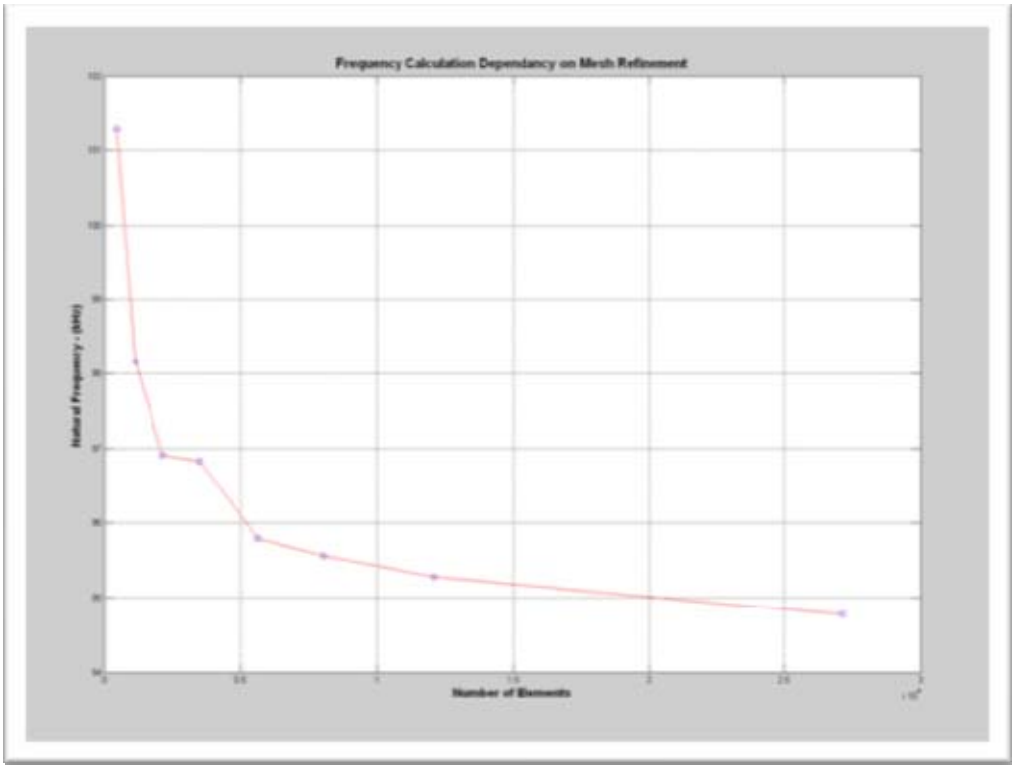


Figure 28: Dependence of solution on mesh refinement with MATLAB

Another application, as was mentioned in the introduction to this section, is incorporating mathematical relationships that are not supported in COMSOL. This is best illustrated in the example of the ideal hyperbolic potential. [35] A model with boundary conditions similar to that of Figure 13 was introduced as a two-dimensional model in COMSOL and converted to MATLAB. The AC/DC model was solved for the potential field. The solution can then be compared to the ideal case, represented as a mathematical equation. [38] Figure 29 shows the model solution and the integration of the ideal hyperbolic geometry for a visual comparison in the MATLAB environment.

Overall, customization in MATLAB scripting allows for flexibility and versatility of COMSOL models. Case studies also prove to verify and instill confidence in models by illustrating the behavior of the device in a wide range of situations. The ability to incorporate new technology into existing models provides the functionality and performance necessary to investigate novel concepts under the proposed process and contributes immensely to the efforts of SCHETCH.

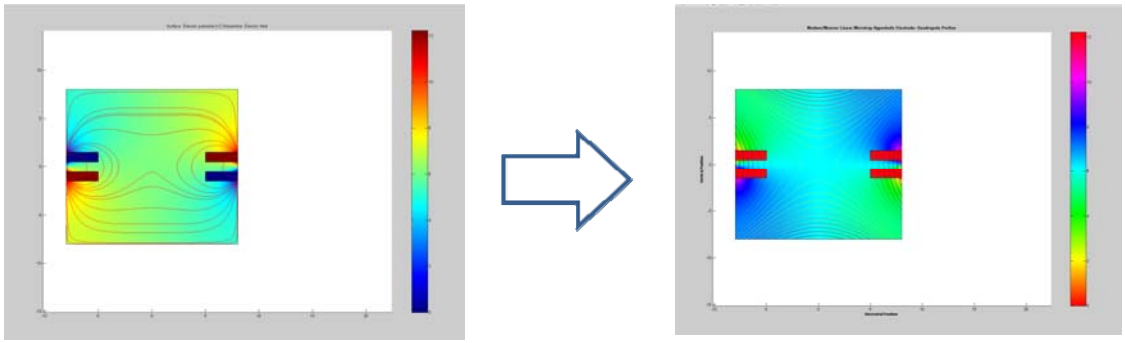


Figure 29: Model comparison of solution to ideal case for hyperbolic potential field

5.2.4 Circuit Models

Circuit analysis of models adds a mode of functionality for ultimate implementation into a systems model. COMSOL Multiphysics recognizes circuits via an interface with SPICE. SPICE is a general purpose circuit simulation program that is used in integrated circuits (ICs) to analyze circuit behavior and performance. [39]

COMSOL and its SPICE import allows for definition of circuit elements, such as resistors, capacitors, sources, and nodes. Nodes are then assigned to the respective physical components in the model and incorporated as boundary conditions. This allows for definition of the model as a component of a circuit, and potentially as an element in a larger control circuit or system circuit. An example of a control system is found below in the control circuit used in experiments by the Maryland group. [41] A smaller sub-circuit may also be defined and implemented from individual components of the model. Such an example exists in the investigation of RF heating by the London Group. [33]

Though a promising feature and integral step in the modeling and simulation hierarchy, circuit modeling in SPICE needs to be further investigated for its adaptability. More knowledge on the implementation of models in the SPICE environment also needs to be obtained to investigate all of its functionality.

5.2.5 Ion Trap Concluding Remarks

The initial finite element modeling of ion traps in SolidWorks and COMSOL has shown that commercially available M&S software can play a role in the analysis and development of ion trap concepts. Further work is needed to understand additional characteristics of ion traps such as RF heating and “breakdown” voltages. SPICE could also play a role in understanding the control circuitry required for ion traps and aid in comparing the characteristics of different design concepts.

In order to implement a physically-functioning quantum information processor, knowledge of the performance of the entire system including ion trap devices, control circuitry, and support devices is necessary. Even with the initial success, the question remains whether existing M&S tools and techniques such as VHDL can be used to properly model a quantum computer design, or do new M&S paradigms need to be developed? If VHDL can be used to model new alternative computing processes than comparison with standard computing processes is possible. It would also imply that there is an increased likelihood of integrating new alternative computing concepts with the current state-of-the-art in computer technology.

6.0 CLOSING REMARKS

An overview of the progress that has been made on the project has been presented. While several alternative computing concepts were examined under this project, a majority of the hands-on experience to date was focused on examining quantum computing concepts. It was found that commercially available three dimensional M&S software tools can be used to analyze concepts for physical components of quantum computing concepts. A process for modeling and simulation was defined, but more work however, is needed to implement SPICE type models and understand how to conduct system level models of quantum computing concepts. Several gaps related to M&S were defined throughout the report. The biggest gap was the lack of a clear understanding and proper definition of material properties for modeling structures at the nanoscale. Future work with quantum computing concepts will be conducted under other in-house efforts especially those examining solid state approaches to quantum computing. Work continues under this effort to develop computational tools to exploit structural DNA nanotechnology which will be presented in more detail in future reports.

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8.0 ACRONYMS

a	acceleration, or distance from fixed end
A	cross sectional area of beam
AC	alternating current
AFRL	Air Force Research Laboratory
BioCOMP	Bio-Computation Program
BioFlips	Bio-Fluidic Chips Program
Bio-SPICE	Biological Simulation Program for Intra-Cellular Evaluation
c	damping constant
CAD	computer-aided design
CMOS	Complementary Metal Oxide on Silicon
CTC	core technical competency
DARPA	Defense Advanced Research Projects Agency
DC	direct current
DNA	deoxyribonucleic acid
E	Young's Modulus, or Modulus of Elasticity
ETCH	Establishing Tools for Computing Hybrids Project
FEA	Finite Element Analysis
FEM	Finite Element Method
h	convection heat transfer coefficient
I	moment of inertia
IC	integrated circuit
k	thermal conductivity in heat transfer systems; spring constant in mechanical systems
L	length
m	mass constant
MEMS	microelectromechanical systems
M&S	modeling and simulation
NEMS	nanoelectromechancial systems
P	load
PDE	partial differential equation
q	heat flux
QuIST	Quantum Information Science and Technology
RF	radio frequency
R&D	research and development
SCHETCH	Simulation Concept – How to Exploit Tools for Computing Project
SIMBIOSYS	Simulation of Biological Systems Program
SPICE	Simulation Program with Integrated Circuit Emphasis
SWCNT	Single Walled Carbon Nanotube
t	depends on context; time, temperature, beam thickmess
T	temperature
v	velocity
V	voltage
VHSIC	Very High Speed Integrated Circuit

ACRONYMS - Continued

VHDL	VHSIC Hardware Description Language
VLSI	Very Large Scale Integration
w	width of beam
x	displacement
ε	emissivity
f_n	natural frequency
λ	electron/phonon mean free path
ρ	density
σ	Boltzmann's Constant